Supporting Information for "**Electrophilic, Ambiphilic, and Nucleophilic C-H Bond Activation: Understanding the Electronic Continuum of C-H Bond Activation Through Transition-state and Reaction Pathway Interaction Energy Decompositions**"

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Explanation of Truncated ligands.
For **7a** and **7b** truncated acac ligands were used (1,3-propanedialate). For **9** the pinacolborate group was truncated and for **11**-**13** pincer complexes PMe_2 was used rather than PBu_2.

Referece 19. QChem 3.1.0.2-serial ALMO version Full Reference
Y. Shao, L. Fusti-Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko,S. V. Levchenko, D. P. O'Neill, R. A. DiStasio Jr., R. C. Lochan, T. Wang, G. J. O. Beran, N. A. Besley, J. M. Herbert, C. Y. Lin, T. Van Voorhis, S. H. Chien, A. Sodt, R. P. Steele, V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson, B. Austin, J. Baker, E. F. C. Byrd, H. Dachsel, R. J. Doerksen, A. Dreuw, B. D. Dunietz, A. D. Dutoi, T. R. Furlani, S. R. Gwaltney, A. Heyden, S. Hirata, C.-P. Hsu, G. Kedziora, R. Z. Khaliullin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang, I. Lotan, N. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek, Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill, A. C. Simmonett, J. E. Subotnik, H. L. Woodcock III, W. Zhang, A. T. Bell, A. K. Chakraborty, D. M. Chipman, F. J. Keil, A. Warshel, W. J. Hehre, H. F. Schaefer III, J. Kong, A. I. Krylov, P. M. W. Gill, M. Head-Gordon, Q-Chem, Version 3.1, Q-Chem, Inc., Pittsburgh, PA (2007).

Additional authors for Version 3.1:
Z. Gan, Y. Zhao, N. E. Schultz, D. Truhlar, E. Epifanovsky and M. Oana.

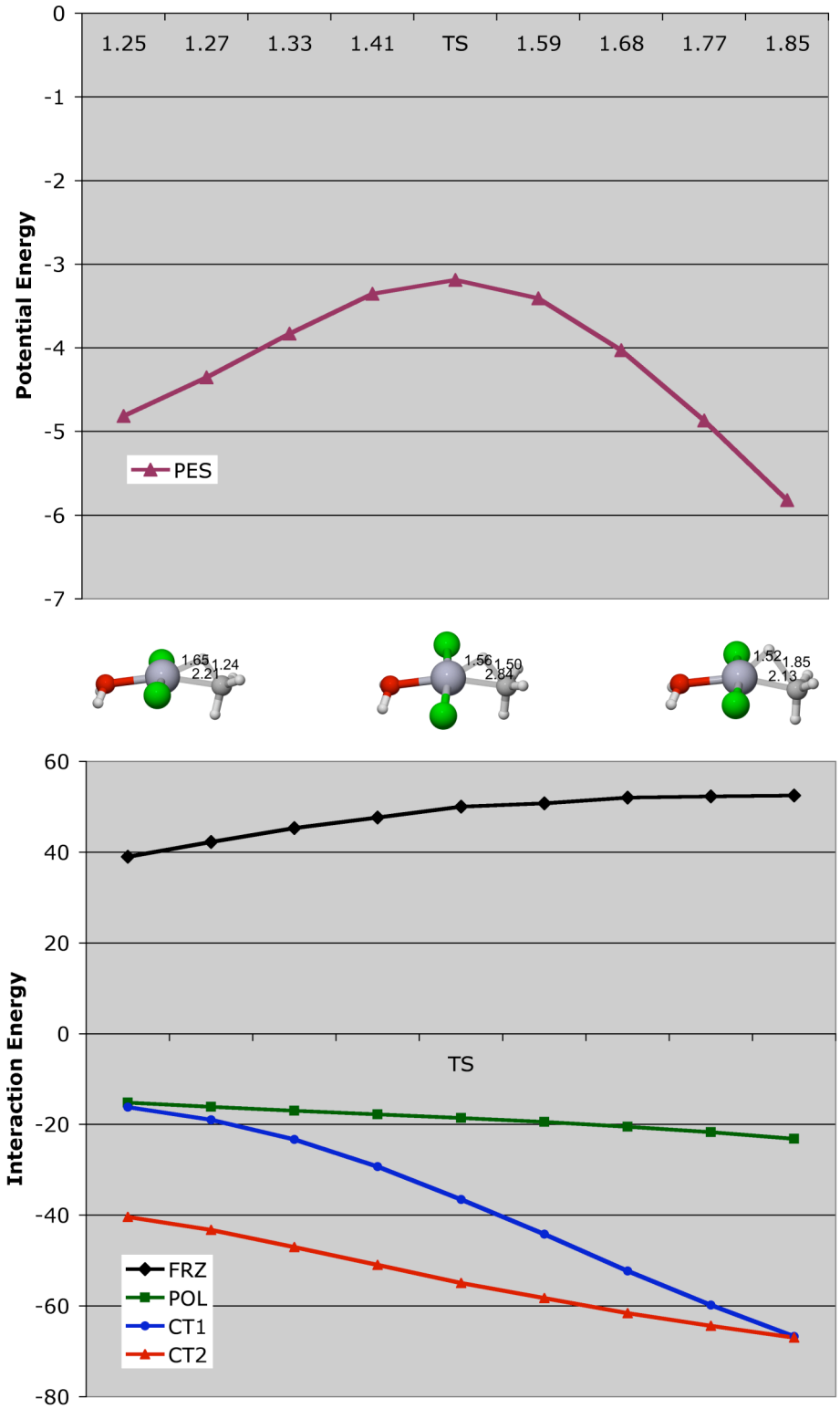

Figure S1. Potential (top, PES) and interaction energy (bottom) surfaces along the IRC for methane C-H bond activation by [$PtCl_2(H_2O)$].

XYZ coordinates and absolute energies (au) of transitions states

1-TS: E = -1147.3989109142

2 1

Pt	1.513030	0.015145	1.511772
N	3.535138	-0.181326	2.375224
N	1.730749	-2.094547	1.637854
N	5.055753	-1.802576	3.074041
N	3.291848	-3.761648	2.353282
Cl	1.578730	2.314806	1.577738
C	3.865471	-1.458639	2.543796
C	2.913122	-2.512611	2.155217
C	5.960102	-0.871926	3.457350
C	5.642149	0.469124	3.295740
C	4.398495	0.788545	2.741981
C	2.424260	-4.727876	2.014793
C	1.172561	-4.409693	1.479706
C	0.854698	-3.063231	1.302730
H	6.895300	-1.231808	3.876023
H	6.340505	1.244400	3.592568
H	4.060270	1.810389	2.579982
H	2.738950	-5.754825	2.177949
H	0.461017	-5.182283	1.207651
H	-0.099720	-2.751137	0.895215
H	5.232624	-2.809920	3.172275

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0 1

C	0.031066	0.148642	-0.070959
H	-0.030417	0.074837	1.654318
H	0.770015	0.133245	-0.875143
H	-0.641581	-0.706448	-0.106334
H	-0.498517	1.097454	-0.029464

2a-TS: E = -1156.5496317793

Pt	-1.498411	2.096189	2.746966
Cl	-0.778472	1.648518	4.953466
Cl	-2.077957	2.768419	0.555144
O	-1.034442	4.161012	3.143182
H	-0.327370	4.221591	3.805666
H	-0.763777	4.604552	2.323112

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0 1

C	-1.319026	0.026702	2.158330
H	-2.442337	0.856374	2.692964
H	-1.167808	-0.599824	3.034293
H	-2.061686	-0.376570	1.468277
H	-0.388274	0.199093	1.616472

2b-TS: E = -1540.4375572805

-1 1

Pt	0.004314	2.189067	0.114367
Cl	1.371154	1.977659	2.065939
Cl	-1.396745	2.277381	-1.822880
Cl	0.483304	4.519110	-0.045750

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0 1

C	0.101714	0.026546	-0.125141
H	-0.846269	0.980724	0.626859
H	0.351196	-0.514667	0.787549
H	-0.734912	-0.415217	-0.667058
H	0.975771	0.075430	-0.777442

3-TS: E = -1574.5123522304

Au	-0.752156	-1.864906	1.859711
S	-0.235307	0.225404	0.120932
O	-0.491141	0.116850	1.746339
O	1.136782	0.629776	-0.122277
O	-0.408372	-1.371548	-0.091001
O	-1.339041	0.944004	-0.488440
O	-1.011044	-3.930235	1.583396
S	-0.525161	-4.896377	2.682662
O	0.365438	-5.927765	2.197752
O	-1.889608	-5.582392	3.227943
O	-0.074497	-4.069165	3.854871
H	-2.040211	-6.401919	2.724923

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0 1

C	-1.258055	-1.676780	4.054369
H	-0.786796	-0.701241	4.156820
H	-0.604574	-2.806966	3.796817
H	-1.092633	-2.198322	5.012709
H	-2.339124	-1.620923	3.925773

4-TS: E = -1566.4827298308

0 1

Pd	0.009148	-0.081978	-0.041875
S	0.009928	-0.006247	2.661607
O	1.186117	0.015154	1.673805
O	-0.079835	1.507755	3.233958
O	-1.192392	-0.169541	1.757516
O	0.144401	-0.895879	3.798024
O	-1.451891	-0.238911	-1.509782
S	-1.346538	0.735116	-2.676186

O	-2.452023	1.663725	-2.820031
O	-1.311747	-0.217435	-3.994157
O	0.046687	1.329880	-2.646689
H	-2.199665	-0.196843	-4.389913
H	0.003723	1.453540	4.201076

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0 1

C	1.788503	-0.190449	-1.302837
H	2.496417	0.209027	-0.578797
H	0.786519	0.625028	-1.817343
H	2.120342	0.117967	-2.304785
H	1.783298	-1.282149	-1.321534

5-TS: E = -1955.2765936641

0 1

Rh	-0.025235	-0.004938	0.014297
C	-0.005439	-0.027069	1.941023
O	0.311800	-0.033600	3.036627
C	0.157611	-1.979816	-0.123385
O	0.348945	-2.924359	0.540850
O	-2.053812	-0.262359	-0.138919
C	-2.720212	-0.221169	0.963280
O	-2.285158	-0.104336	2.105371
C	-4.247877	-0.351489	0.722528
F	-4.675040	0.632944	-0.083197
F	-4.515981	-1.531426	0.135056
F	-4.921116	-0.286532	1.872701
O	-0.461180	2.106836	-0.033596
C	0.508905	2.863364	0.235657
O	1.682870	2.497552	0.490250
C	0.193281	4.377411	0.255141
F	1.284385	5.100792	0.522324
F	-0.291758	4.754414	-0.938017
F	-0.731683	4.631314	1.194715
O	-0.085288	-0.130366	-2.103966
C	-0.159300	-1.317603	-2.455676
O	-0.068377	-2.342463	-1.677293
C	-0.367989	-1.671054	-3.945591
F	0.647968	-2.438619	-4.363509
F	-0.416812	-0.567175	-4.687106
F	-1.513218	-2.348741	-4.080610

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0 1

H	1.761506	1.146398	0.251050
C	2.313701	-0.028256	-0.060514
H	3.171409	0.631167	0.140646

H	2.448883	-0.876000	0.608433
H	2.397684	-0.315519	-1.107743

6a-TS: E = -1026.0264551946

0 1

Ru	0.001866	0.000635	0.000204
N	-0.003196	-0.002336	2.183540
C	0.062941	0.014005	-1.868793
N	2.027125	-0.596411	0.182877
N	0.735179	1.986586	0.159899
N	1.686886	2.255127	1.091816
N	1.067259	0.535802	2.820783
N	2.819358	0.014000	1.101356
B	2.240350	1.131048	2.000103
H	3.084768	1.562751	2.734126
O	0.120637	0.028640	-3.024682
O	-0.987240	-1.897664	-0.005740
H	-0.885755	-2.245039	0.891896
C	2.008645	3.567570	1.043655
H	2.752491	3.971954	1.714187
C	1.249773	4.171590	0.053470
H	1.263042	5.208054	-0.246854
C	-0.843829	-0.440961	3.129745
H	-1.780855	-0.903560	2.853756
C	-0.314995	-0.187028	4.403643
H	-0.754117	-0.418854	5.361795
C	4.046570	-0.553833	1.085008
H	4.819881	-0.203547	1.752778
C	4.054306	-1.557200	0.128083
H	4.876174	-2.202279	-0.142431
C	0.465708	3.134751	-0.473867
H	-0.265219	3.156829	-1.269343
C	0.899833	0.435831	4.157367
H	1.652580	0.814408	4.833204
C	2.758770	-1.545332	-0.411384
H	2.320656	-2.161068	-1.183499

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0 1

C	-2.332660	0.381187	0.027072
H	-1.743566	-0.863281	0.041374
H	-2.010950	1.427113	0.011786
H	-2.922707	0.262702	0.943044

6b-TS: E = -1006.1547764977

0 1

Ru	-0.097506	-0.005873	-0.073317

N	-0.053663	0.001502	2.107207
C	-0.179243	0.021642	-1.936208
N	-1.540879	1.526699	0.137819
N	-1.762660	-1.375271	0.148093
N	-2.692567	-1.108288	1.101453
N	-1.231822	0.071301	2.776604
N	-2.513475	1.398516	1.077190
B	-2.563868	0.149043	1.990782
H	-3.491311	0.223578	2.747933
O	-0.234884	0.058548	-3.094582
N	1.700385	1.123998	-0.029123
H	1.908732	1.677782	-0.852300
C	-3.641347	-2.071845	1.095151
H	-4.467920	-2.029585	1.789002
C	-3.324802	-2.993164	0.109540
H	-3.872961	-3.882119	-0.162267
C	0.919363	-0.036697	3.024417
H	1.953060	-0.095053	2.714466
C	0.370348	0.008441	4.314800
H	0.893626	-0.008015	5.258528
C	-3.300455	2.497874	1.063416
H	-4.131772	2.582416	1.747602
C	-2.831993	3.363368	0.087048
H	-3.233622	4.326791	-0.187169
C	-2.135821	-2.508223	-0.456854
H	-1.540676	-2.913000	-1.263164
C	-0.999497	0.076628	4.107473
H	-1.821259	0.128166	4.806535
C	-1.722718	2.706024	-0.465746
H	-1.057982	3.015996	-1.258825
H	1.742598	1.711299	0.797430

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0 1

C	1.694802	-1.588583	-0.076796
H	1.843600	-0.251912	-0.040189
H	0.842557	-2.274893	-0.069372
H	2.274909	-1.811730	0.825534
H	2.288263	-1.811331	-0.968552

6c-TS: E = -990.0968141236

0 1

Ru	0.597923	-0.115794	0.277977
N	0.682832	-0.525202	-1.877311
C	0.553828	0.276098	2.098692
C	1.188873	-2.226295	0.681900
N	0.182158	1.945310	-0.341467

N	2.687178	0.493947	0.028617
N	3.032047	1.224034	-1.062921
N	1.315981	0.361478	-2.686952
N	0.874059	2.468685	-1.385731
B	1.964599	1.639259	-2.102259
H	2.468195	2.285108	-2.979517
O	0.531845	0.524647	3.231192
H	2.039853	-2.107355	1.354328
H	1.525786	-2.620614	-0.277493
H	0.520362	-2.962850	1.145865
C	4.359026	1.482498	-1.036546
H	4.819734	2.056536	-1.827012
C	4.896812	0.905918	0.104240
H	5.925455	0.925110	0.430636
C	0.241933	-1.521461	-2.656155
H	-0.299515	-2.350636	-2.223257
C	0.590199	-1.283679	-3.994060
H	0.376231	-1.899382	-4.854257
C	0.456441	3.733225	-1.620310
H	0.896461	4.315534	-2.416488
C	-0.535890	4.046100	-0.703651
H	-1.079062	4.974206	-0.611036
C	3.802753	0.298361	0.739505
H	3.766998	-0.259424	1.664636
C	1.271892	-0.075768	-3.964910
H	1.726484	0.501921	-4.756211
C	-0.668894	2.887957	0.077871
H	-1.325408	2.694143	0.914410

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0 1

H	-0.219327	-1.466136	0.524339
C	-1.569514	-0.642315	0.275670
H	-1.856431	-0.818496	-0.762182
H	-1.986911	-1.442202	0.899347
H	-2.011947	0.293283	0.621250

7a-TS: E = -906.8773604543

Ir1	0.2027371143	0.0775061700	0.0882566957
O2	0.9282617775	-0.5935255486	1.9216997229
C3	1.0896574730	-1.7498652679	-1.9997180364
O4	1.1813657936	-1.5073482341	-0.7532140406
H5	1.6919811430	-2.6041732097	-2.3308273573
C6	-0.3184522634	2.8229439633	0.9275697741
O7	-0.7650325314	1.6282997555	1.0142450529
H8	-0.9452836136	3.5675848230	1.4318862355
C9	1.7766193115	2.4926600289	-0.3840378061

C10	0.8408237924	3.2815866941	0.2987173230
H11	2.6489453842	3.0036739019	-0.8090847115
H12	1.0400291700	4.3461153065	0.3505582286
O13	1.7646241183	1.2360313626	-0.5830069842
C14	-0.5024759787	0.0150440689	-2.7520487350
C15	0.3291415180	-1.0865901799	-2.9712978050
H16	-1.0445140167	0.4159293580	-3.6170976581
H17	0.3899707188	-1.4643446393	-3.9858854404
O18	-0.7341437459	0.6360542348	-1.6614205170
C19	-1.4362182559	-1.3107138371	0.9217295053
H20	-0.3035880616	-1.0326556121	1.5508103732
H21	0.7707700451	0.1192261129	2.5600432645
H22	-1.9531532266	-1.0488133597	-0.0053210799
H23	-1.3016829399	-2.3958382934	0.9216180056
H24	-2.0898707420	-0.9794365720	1.7345607512

7b-TS: E = -718.2813730924

0 1

Ir	0.000000	0.000000	0.416503
O	-0.199340	2.045004	0.426169
O	1.358283	0.022906	-1.268708
O	-1.358283	-0.022906	-1.268708
O	0.199340	-2.045004	0.426169
C	-1.828787	-0.107282	1.520014
C	0.359591	2.775543	-0.458097
C	1.203039	2.416980	-1.513193
C	1.632663	1.122582	-1.840013
C	-1.632663	-1.122582	-1.840013
C	-1.203039	-2.416980	-1.513193
C	-0.359591	-2.775543	-0.458097
H	1.561249	3.223973	-2.142829
H	-1.561249	-3.223973	-2.142829
H	-1.903793	-1.030372	2.098158
H	-1.965536	0.761164	2.166662
H	-2.582253	-0.089810	0.731296
H	0.131253	3.842798	-0.348916
H	2.305848	1.037883	-2.705567
H	-2.305848	-1.037883	-2.705567
H	-0.131253	-3.842798	-0.348916

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0 1

C	1.828787	0.107282	1.520014
H	2.582253	0.089810	0.731296
H	1.903793	1.030372	2.098158
H	1.965536	-0.761164	2.166662
H	0.000000	0.000000	1.964117

8a-TS: E = -825.2680399391

1 1

Ir	0.007926	-0.054549	-0.454093
P	-2.259772	0.044939	0.072664
C	-0.408828	1.640893	-1.725534
C	1.685090	-1.161387	0.796505
C	0.916491	-0.383274	1.691629
C	1.015826	0.998377	1.279744
C	1.920194	1.051287	0.164158
C	2.300218	-0.277356	-0.164922
C	-2.798063	1.659187	0.764146
C	-3.437469	-0.264081	-1.304103
C	-2.773768	-1.173110	1.352499
H	0.431842	1.771310	-2.408435
H	-1.315662	1.531626	-2.321045
H	-0.497082	2.525617	-1.092211
H	-3.850061	-1.096780	1.535000
H	-2.544573	-2.190097	1.024069
H	-2.243493	-0.980180	2.288000
H	-3.328873	-1.284767	-1.677058
H	-4.462132	-0.132608	-0.944145
H	-3.262207	0.432764	-2.126215
H	-2.227705	1.885741	1.668125
H	-2.631840	2.454995	0.035046
H	-3.862378	1.624115	1.015419
H	2.224603	1.946060	-0.361168
H	2.971580	-0.570695	-0.960157
H	1.791256	-2.237898	0.820026
H	0.353909	-0.757037	2.535847
H	0.600842	1.851231	1.798166

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0 1

C	-0.456287	-1.984898	-1.563113
H	-0.126109	-0.551627	-1.971214
H	0.474156	-2.427903	-1.914594
H	-0.853241	-2.570851	-0.734668
H	-1.185652	-1.981028	-2.374106

8b-TS: E = -804.6834085146

0 1

Rh	-0.019530	-0.056396	-0.004513
P	-0.028670	-0.053716	2.247013
C	1.354986	0.271495	-1.989394
C	2.221489	-0.051208	-0.938746
C	1.817843	-1.347964	-0.435017
C	0.791352	-1.868194	-1.282063

C	0.441571	-0.832683	-2.182313
H	1.349215	1.194058	-2.555408
H	3.020164	0.562417	-0.545313
H	2.330100	-1.901752	0.342251
H	0.325751	-2.840468	-1.203751
H	-0.323014	-0.886145	-2.946513
C	-0.384167	-1.681309	3.062698
H	-1.384525	-2.014607	2.774397
H	0.332850	-2.426926	2.708745
H	-0.324569	-1.614485	4.155228
C	-1.215506	1.052321	3.139221
H	-1.039921	2.092355	2.852288
H	-2.241320	0.790743	2.866524
H	-1.101920	0.956331	4.224101
C	1.573677	0.407811	3.058796
H	1.510897	0.339114	4.150706
H	2.363452	-0.259704	2.704246
H	1.842043	1.429127	2.776389

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C	-1.562104	1.532959	-0.231614
H	-2.342129	1.729305	0.508149
H	-0.825296	2.337235	-0.168870
H	-1.602997	0.098476	0.030310
H	-2.012084	1.531115	-1.226218

9-TS: E = -782.5595094919

0 1

W	-0.257980	0.076191	0.141452
C	-1.628379	1.338288	0.800859
O	-2.412934	2.096343	1.209160
C	-1.479858	0.222932	-1.388729
O	-2.169254	0.325377	-2.327426
B	-1.072307	-1.960321	-0.539716
C	1.994794	0.056671	1.087684
C	2.009095	-0.721555	-0.103948
C	1.685076	0.140556	-1.192334
C	1.471834	1.455642	-0.669321
C	1.658867	1.395234	0.746395
H	2.188524	-0.311362	2.086703
H	2.218567	-1.779161	-0.178227
H	1.638344	-0.147266	-2.233198
H	1.247890	2.343255	-1.244319
H	1.577565	2.225230	1.435050
O	-0.253395	-2.804658	-1.273790
O	-2.346984	-2.470535	-0.399113

C	-2.457058	-3.654281	-1.205593
H	-2.935807	-4.447849	-0.623764
H	-3.087016	-3.430827	-2.074415
C	-1.002727	-3.988842	-1.605653
H	-0.597005	-4.835631	-1.038788
H	-0.891293	-4.201106	-2.673193

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C	-0.966676	-0.824575	2.308209
H	-2.049256	-0.808530	2.415306
H	-0.513609	-0.055742	2.931953
H	-0.586620	-1.796062	2.638531
H	-0.771012	-1.400003	0.921650

10-TS: E = -514.0143478632

0 1

Sc	0.002817	0.185049	0.000010
C	-0.037533	2.114450	1.432155
C	1.611433	-1.746642	0.000045
C	1.906828	-0.968182	-1.146930
C	1.906624	-0.968303	1.147158
C	2.410352	0.285754	-0.707342
C	2.410228	0.285678	0.707792
C	-2.513402	0.441782	-0.000072
C	-2.182740	-0.322654	1.146619
C	-2.182624	-0.322350	-1.146933
C	-1.636161	-1.555546	0.710633
C	-1.636088	-1.555357	-0.711219
H	0.035175	1.361361	2.234692
H	0.805143	2.800650	1.569217
H	-0.969796	2.665842	1.593979
H	1.214954	-2.753874	-0.000045
H	1.789639	-1.283473	-2.177379
H	1.789257	-1.283703	2.177553
H	2.734812	1.098658	-1.343457
H	2.734575	1.098514	1.344049
H	-2.934208	1.439021	0.000039
H	-2.316507	-0.013104	2.176084
H	-2.316289	-0.012522	-2.176327
H	-1.293502	-2.361365	1.347783
H	-1.293363	-2.361006	-1.348549

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H	-0.028038	2.071554	0.000079
C	-0.037315	2.114559	-1.431999
H	0.035573	1.361534	-2.234578

H	0.805369	2.800791	-1.568858
H	-0.969567	2.665937	-1.593937

11-TS: E = -1312.7733786876

0 1

Ir	-0.080556	0.002703	-0.001656
N	-0.380963	0.025200	-2.070640
P	0.038249	-2.300613	-0.343012
P	0.013403	2.278245	-0.291182
C	-0.268380	-1.187334	-2.774403
C	-0.071306	-2.382028	-2.094339
H	-0.001949	-3.310891	-2.651399
C	-0.606730	1.191887	-2.754887
C	1.687767	3.007040	-0.578146
H	2.268136	2.965735	0.347544
H	2.204103	2.404539	-1.329722
H	1.627832	4.046195	-0.919220
C	-0.797755	3.558707	0.769416
H	-0.733364	4.556996	0.324040
H	-1.848656	3.295228	0.915783
H	-0.312393	3.580365	1.749509
C	1.595954	-3.141497	0.208457
H	2.452023	-2.588047	-0.183379
H	1.657220	-3.160689	1.301620
H	1.634897	-4.171170	-0.163685
C	-1.240462	-3.418603	0.407059
H	-2.233375	-3.056856	0.130121
H	-1.122651	-4.445511	0.043959
H	-1.156141	-3.419969	1.499010
C	-0.358007	-1.134483	-4.209817
C	-0.541433	0.048566	-4.865408
H	-0.260761	-2.067778	-4.755088
H	-0.594305	0.067925	-5.951252
C	-0.673082	1.252782	-4.130217
H	-0.853352	2.199932	-4.625217
C	-0.844240	2.437617	-1.928602
H	-1.915047	2.518478	-1.695972
H	-0.560902	3.339151	-2.481737

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0 1

C	-0.242561	-0.081841	2.252086
H	0.822889	-0.048271	1.353284
H	-1.330614	-0.144768	2.152726
H	0.108691	-0.963528	2.795267
H	0.012215	0.810530	2.828454

12-TS: E = -1368.5869672431

0 1

Ir	-0.001191	0.008026	0.049287
C	-0.346382	-0.013996	-1.967293
P	-0.117894	-2.245036	-0.331817
P	0.123489	2.243229	-0.423682
C	-0.529283	-1.213730	-2.672464
C	-0.402292	1.168844	-2.721154
C	1.721350	3.141259	-0.313938
H	1.986715	3.288051	0.737533
H	2.496535	2.534553	-0.786801
H	1.659999	4.112286	-0.814164
C	-1.080696	3.469197	0.229499
H	-0.988765	4.426311	-0.292556
H	-2.091284	3.077625	0.093089
H	-0.906112	3.619918	1.299349
C	1.372627	-3.306828	-0.178525
H	2.208717	-2.810817	-0.676079
H	1.622568	-3.434544	0.879299
H	1.203861	-4.286959	-0.634519
C	-1.445899	-3.305769	0.369434
H	-2.409608	-2.815709	0.212509
H	-1.456745	-4.289526	-0.109305
H	-1.287107	-3.426412	1.445593
C	-0.774724	-1.255589	-4.044289
C	-0.832400	-0.045179	-4.741196
H	-0.911840	-2.206431	-4.548370
H	-1.023027	-0.057117	-5.810884
C	-0.644877	1.179730	-4.094188
H	-0.681215	2.117841	-4.637691
O	-0.195409	2.379583	-2.072352
O	-0.451469	-2.412893	-1.974445

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0 1

C	-0.106007	0.057634	2.314237
H	1.043015	-0.023266	1.284630
H	-1.200266	0.116296	2.298876
H	0.190313	-0.834979	2.870116
H	0.285671	0.933598	2.836567

13a-TS: E = -1296.7394881671

0 1

Ir	-0.008291	0.003998	0.029011
C	-0.350862	-0.009400	-2.026832
P	0.059526	-2.270119	-0.296831
P	-0.021646	2.275358	-0.345037

C	-0.168434	-1.184553	-2.805152
C	-0.791377	1.155855	-2.712015
C	1.608267	3.038715	-0.764822
H	2.269166	2.992912	0.104895
H	2.063583	2.458036	-1.570374
H	1.497319	4.081721	-1.081254
C	-0.757966	3.531301	0.796284
H	-0.757495	4.532313	0.352279
H	-1.785099	3.244500	1.036111
H	-0.184998	3.558753	1.727856
C	1.334187	-3.355069	0.486496
H	2.324919	-2.929751	0.306325
H	1.169162	-3.391275	1.567366
H	1.299677	-4.374616	0.088301
C	-1.496580	-3.237277	-0.028822
H	-2.300893	-2.768143	-0.601117
H	-1.386532	-4.280054	-0.346140
H	-1.769317	-3.211109	1.029583
C	-0.430694	-1.193674	-4.178942
C	-0.860266	-0.032952	-4.822953
H	-0.287906	-2.106950	-4.753747
H	-1.056862	-0.042629	-5.892040
C	-1.032748	1.141090	-4.089886
H	-1.365430	2.047683	-4.593066
C	-1.006386	2.430849	-1.915666
H	-2.058387	2.533591	-1.616446
H	-0.748103	3.332871	-2.485115
C	0.367472	-2.430272	-2.125112
H	-0.054767	-3.355394	-2.538444
H	1.456453	-2.494382	-2.251165

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0 1

C	-0.137011	0.038380	2.290053
H	1.020784	0.009429	1.272784
H	-1.232771	0.009529	2.273209
H	0.224175	-0.822805	2.859483
H	0.180500	0.946954	2.808589

13b-TS: E = -1301.5248098625

0 1

Rh	0.000146	0.005888	0.082525
C	-0.346698	-0.008210	-2.020665
P	0.091194	-2.273471	-0.301976
P	-0.021510	2.283178	-0.347141
C	-0.121069	-1.170241	-2.801355
C	-0.832108	1.142858	-2.690613

C	1.592103	3.008540	-0.882055
H	2.299722	2.985610	-0.049028
H	1.994430	2.394473	-1.691153
H	1.476039	4.040702	-1.229963
C	-0.689027	3.594275	0.776336
H	-0.708606	4.575173	0.289847
H	-1.703284	3.327303	1.085269
H	-0.066852	3.656573	1.673524
C	1.299178	-3.421841	0.496507
H	2.309348	-3.022872	0.373296
H	1.087051	-3.485963	1.567471
H	1.252713	-4.426746	0.063666
C	-1.502031	-3.203803	-0.139876
H	-2.265140	-2.699182	-0.737912
H	-1.403249	-4.239614	-0.482614
H	-1.826180	-3.200608	0.904534
C	-0.392396	-1.184669	-4.174605
C	-0.873794	-0.037449	-4.806587
H	-0.217755	-2.087297	-4.757348
H	-1.078958	-0.049484	-5.874123
C	-1.085610	1.126711	-4.067992
H	-1.454669	2.021215	-4.566535
C	-1.075703	2.402824	-1.878593
H	-2.119455	2.456216	-1.538582
H	-0.879628	3.320592	-2.448085
C	0.472178	-2.389998	-2.121160
H	0.127224	-3.336361	-2.557523
H	1.567789	-2.378592	-2.208606

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0 1

C	-0.237301	0.021024	2.236402
H	1.194856	0.036591	1.062315
H	-1.335912	-0.017693	2.231944
H	0.145074	-0.842039	2.788366
H	0.081550	0.927719	2.757297